

1,3-diphenylpropane-1,2-diol
5381-84-0 | DTXSID50281584

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.66e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.61e-01

Confidence level: 3.09e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methylcyclopentane</div> <div>Measured: 9.75e-11</div> <div>Predicted: 80.1</div>	<div>Image not found</div> <div>Hydroprene</div> <div>Measured: 3.39e-09</div> <div>Predicted: 8.80e-04</div>	<div>Image not found</div> <div>2-Propanone, 1,3-diphenyl-</div> <div>Measured: 7.53e-06</div> <div>Predicted: 3.07e-04</div>
<div>Image not found</div> <div>Ethylenediaminetetraacetic acid</div> <div>Measured: 1.40e-06</div> <div>Predicted: 2.81e-12</div>		